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The electronic structure of catalysts by X-ray emission based methods: Fundamental investigations and applications

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The catalytic activity of catalysts is commonly guided by the interplay of geometric and electronic effects at the active center. It are the highest occupied (HOMO) and lowest unoccupied (LUMO) states that interact with the substrate in dependence of the coordination geometry. Knowledge about these three "structure factors" is therefore a key to understand catalytic mechanisms and the working principle of catalysts. X-ray emission methods using synchrotron radiation allow the determination of all three parameters in one experiment under almost any reaction conditions, like high pressures and temperatures, low catalyst concentration etc.: HERFD-XANES (High-energy resolution fluorescence detected X-ray absorption near edge structure) makes the LUMO states accessible by $1s \rightarrow nd$ transitions, while with valence-to-core XES (X-ray emission spectroscopy) and the underlying $nd \rightarrow 1s$ emission, information about the HOMOs is yielded. The two-dimensional combination of both, called valence-to-core RIXS (Resonant inelastic X-ray scattering) scans the individual $nd \rightarrow 1s$ emissions in dependence of the $1s \rightarrow nd$ excitations, by which analogue information to optical absorption spectroscopy is provided, but in an element selective manner.

With the present contribution, these methods will be introduced on a common level, followed by demonstrating their potential with measurements on iron carbonyls, which serve as model compounds for catalytically active substances or intermediates in many catalytic reactions (e.g. CO-oxidation, catalytic water splitting, biomass conversion etc.). Ferrites $MFeO_3$ as an example for heterogeneous catalysts, used in methane combustion will be discussed with special emphasis on oxidation states and site selective structural investigations of metal centers. The talk will be concluded by presentation of recent results about HERFD-XANES measurements on different cobalt compounds used for CO-oxidation and other selected examples.

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Heterogeneous catalysis

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Talk

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